# Fidelity approach to quantum phase transitions: finite size scaling for quantum Ising model in a transverse field

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We analyze the scaling parameter, extracted from the fidelity for two different ground states, for the one-dimensional quantum Ising model in a transverse field near the critical point. It is found that, in the thermodynamic limit, the scaling parameter is singular, and the derivative of its logarithmic function with respect to the transverse field strength is logarithmically divergent at the critical point. The scaling behavior is confirmed numerically by performing a finite size scaling analysis for systems of different sizes, consistent with the conformal invariance at the critical point. This allows us to extract the correlation length critical exponent, which turns out to be universal in the sense that the correlation length critical exponent does not depend on either the anisotropic parameter or the transverse field strength.

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*Introduction.* An emerging picture arises due to latest advances in quantum information science, which allows us to study quantum phase transitions (QPTs) [1] from the ground state wave functions of many-body systems. One of the well-studied aspects is to unveil the possible role of entanglement in characterizing QPTs [2, 3, 4, 5, 6, 7] (for a review, see [8]). Remarkably, for quantum spin chains, the von Neumann entropy, as a bipartite entanglement measure, exhibits qualitatively different behaviors at and off criticality [4].

On the other hand, the fidelity, another basic notion of quantum information science, has attracted a lot of attention [9, 10, 11] quite recently. In Ref. [10], it has been shown that it may be used to characterize QPTs, which occur in quantum spin chain, regardless of what type of internal order is present in quantum many-body states (either the conventional symmetry-broken orders or exotic QPTs in matrix product systems [12]). The argument is solely based on the basic Postulate of Quantum Mechanics on quantum measurements. Indeed, the basic Postulate of Quantum Mechanics on quantum measurements implies that two non-orthogonal quantum states are not reliably distinguishable [13]. Therefore, any two ground states must be orthogonal due to the occurrence of orders, regardless of what type of QPTs. Conversely, the fact that two ground states are orthogonal implies that they are reliably distinguishable. Therefore, an order parameter, which may be constructed systematically in principle [14], exists for any systems undergoing QPTs. It is the quantitative or qualitative difference unveiled in order parameters that justifies the introduction of the notions of irrelevant and relevant information. To quantify irrelevant and relevant information, the scaling parameter extracted from the fidelity was introduced to characterize QPTs. This establishes an intriguing connection between quantum information theory, QPTs, renormalization group (RG) flows and condensed matter physics.

The fact that any two different ground states are orthogonal for continuous QPTs makes it difficult (if not impossible) to extract physical information solely from ground states themselves. Conventionally, condensed matter physicists and field theorists focus on spectra and correlation functions. Therefore, it is somewhat surprising to see that simply partitioning a system into two parts and quantifying entanglement between them reveal highly nontrivial information about QPTs. The intrinsic irreversibility due to information loss along RG flows may also be revealed solely from ground states [4, 15, 16, 17]. In the fidelity approach [10], it is necessary to put the whole system on a finite chain, and observe how the fidelity scales with system sizes as the thermodynamic limit is approached, in order to extract physical information. The difference between entanglement measures and the fidelity approach lies in the fact that for the former different entanglement measures need to be devised to detect QPTs [7], whereas the latter succeeds to detect QPTs for quantum spin chains, regardless of what order is present. The philosophy behind this is that *bipartite entanglement measures involve partitions and some information is lost due to the fact that the whole is not simply the sum of the parts, whereas in the fidelity approach, a system is treated as a whole from the starting point*.

In this paper, we analyze the scaling parameter, extracted from the fidelity, for the one-dimensional quantum Ising model in a transverse field near the critical point. It is found that, in the thermodynamic limit, the scaling parameter is singular, and the derivative of its logarithmic function with respect to the transverse field strength (the control parameter) is logarithmically divergent at the critical point. A finite size scaling analysis is carried out for systems of different sizes, and the scaling behavior is confirmed numerically, consistent with the conformal invariance at the critical point. This allows us to extract the correlation length critical exponent. We have also performed numerics to confirm the universality, i.e., the correlation length critical exponent does not depend on either the anisotropic parameter or the transverse field strength.

*The fidelity and the scaling parameter for quantum $XY$ spin chain.* The quantum $XY$ spin chain is described by the Hamil-

tonian

$$H=-\sum_{j=-M}^{M}(\frac{1+\gamma}{2}\sigma_j^x\sigma_{j+1}^x+\frac{1-\gamma}{2}\sigma_j^y\sigma_{j+1}^y+\lambda\sigma_j^z). \quad (1)$$

Here $\sigma_j^x, \sigma_j^y$, and $\sigma_j^z$ are the Pauli matrices at the $j$-th lattice site. The parameter $\gamma$ denotes an anisotropy in the nearest-neighbor spin-spin interaction, whereas $\lambda$ is an external magnetic field. The Hamiltonian (1) may be exactly diagonalized [18, 19] as $H=\sum_k \Lambda_k(c_k^\dagger c_k-1)$, where $\Lambda_k=\sqrt{(\lambda-\cos(2\pi k/L))^2+\gamma^2\sin^2(2\pi k/L)}$, with $c_k$ and $c_k^\dagger$ denoting free fermionic modes and $L=2M+1$. The ground state $|\psi\rangle$ is the vacuum of all fermionic modes defined by $c_k|\psi\rangle=0$, and may be written as $|\psi\rangle=\prod_{k=1}^M(\cos(\theta_k/2)|0\rangle_k|0\rangle_{-k}-i\sin(\theta_k/2)|1\rangle_k|1\rangle_{-k}$, where $|0\rangle_k$ and $|1\rangle_k$ are, respectively, the vacuum and single excitation of the $k$-th mode, and $\theta_k$ is defined by $\cos\theta_k=(\cos(2\pi k/L)-\lambda)/\Lambda_k$. Therefore, the fidelity $F$ for two different ground states $|\psi(\lambda,\gamma)\rangle$ and $|\psi(\lambda',\gamma)\rangle$ takes the form:

$$F(\lambda,\lambda';\gamma)=\prod_{k=1}^{M}\cos\frac{\theta_k-\theta_k'}{2}, \quad (2)$$

where the prime denotes that the corresponding variables take their values at $\lambda'$. Obviously, $F=1$ if $\lambda=\lambda'$. Generically, $\cos\frac{\theta_k-\theta_k'}{2}<1$, therefore the fidelity (2) decays very fast when $\lambda$ separates from $\lambda'$.

Now let us introduce a fundamental quantity-the scaling parameter $d(\lambda,\lambda';\gamma)$. For a large but finite $L$, the fidelity scales as $d^L$, with some scaling parameter $d$ depending on $\lambda$ and $\lambda'$, due to the symmetry under translation. Formally, in the thermodynamic limit, $d(\lambda,\lambda')$ may be defined as

$$\ln d(\lambda,\lambda';\gamma)=\lim_{L\to\infty}\ln F(\lambda,\lambda';\gamma)/L. \quad (3)$$

The scaling parameter $d(\lambda,\lambda';\gamma)$ enjoys some properties inherited from the fidelity: (1) symmetry under interchange $\lambda\longleftrightarrow\lambda'$; (2) $d(\lambda,\lambda;\gamma)=1$; and (3) $0\le d(\lambda,\lambda';\gamma)\le 1$.

In the thermodynamic limit, the scaling parameter $d(\lambda,\lambda';\gamma)$ for the quantum XY model takes the form:

$$\ln d(\lambda,\lambda';\gamma)=\frac{1}{2\pi}\int_0^\pi d\alpha\ln\mathcal{F}(\lambda,\lambda';\gamma;\alpha), \quad (4)$$

where

$$\mathcal{F}(\lambda,\lambda';\gamma;\alpha)=\cos[\vartheta(\lambda;\gamma;\alpha)-\vartheta(\lambda';\gamma;\alpha)]/2, \quad (5)$$

with

$$\cos\vartheta(\lambda;\gamma;\alpha)=(\cos\alpha-\lambda)/\sqrt{(\cos\alpha-\lambda)^2+\gamma^2\sin^2\alpha}. \quad (6)$$

A notable feature of the scaling parameter (4) is that, besides $d(\lambda,\lambda';\gamma)=d(\lambda',\lambda;\gamma)$ and $d(\lambda,\lambda;\gamma)=1$, it even detects the duality between two phases $\lambda>1$ and $\lambda<1$ for quantum Ising model in a transverse field ($\gamma=1$) [19], since it satisfies $d(\lambda,\lambda';1)=d(1/\lambda,1/\lambda';1)$.

It has been shown [10] that the scaling parameter $d(\lambda,\lambda';\gamma)$ exhibits a pinch point at $(1,1)$, i.e., an intersection of two singular lines $\lambda=1$ and $\lambda'=1$, for quantum Ising model in a transverse field ($\gamma=1$). In Fig. 1, we plot the scaling parameter $d(\lambda,\lambda';\gamma)$ against $\lambda$ for different values of $\lambda'$ and $\gamma$. One observes the continuity, as it should be for continuous QPTs.

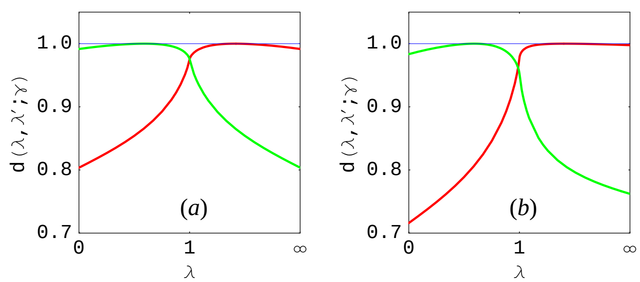


FIG. 1: (color online) The scaling parameter $d(\lambda,\lambda';\gamma)$, extracted from the fidelity for two ground states $|\psi(\lambda)\rangle$ and $|\psi(\lambda')\rangle$ of quantum Ising model in a transverse field, is regarded as a function of $\lambda$ for some fixed values of $\lambda'$ and $\gamma$. It is continuous but not analytic at $\lambda_c=1$. ($a$): the red line is for $\lambda'=2, \gamma=1$, which touches the blue line at $\lambda=2$ and the green line is for $\lambda'=1/2, \gamma=1$, touching the blue line at $\lambda=1/2$. The mirror symmetry between two curves results from the duality. ($b$): the green line is for $\lambda'=1/2, \gamma=1/2$, touching the blue line at $\lambda=1/2$ and the red line is for $\lambda'=2, \gamma=1/2$, touching the blue line at $\lambda=2$. No mirror symmetry for $\gamma\neq 1$.

Let us focus on the quantum Ising universality class with the critical line $\gamma\neq 0$ and $\lambda_c=1$. There is only one (second-order) critical point $\lambda_c=1$ separating two gapful phases: (spin reversal) $Z_2$ symmetry-breaking and symmetric phases. The order parameter, i.e., magnetization $\langle\sigma^x\rangle$ is non-zero for $\lambda<1$, and otherwise zero. At the critical point, the correlation length $\xi\sim|\lambda-\lambda_c|^\nu$ with $\nu=1$ [19]. Our purpose is to extract the correlation length critical exponent by performing a finite size scaling analysis for $d(\lambda,\lambda';\gamma)$.

*Finite size scaling.* In order to quantify the drastic change of the ground state wave functions when the system undergoes a QPT at the critical point $\lambda_c=1$, we evaluate the derivative of $\ln d(\lambda,\lambda';\gamma)$ with respect to $\lambda$. In the thermodynamic limit, $\ln d(\lambda,\lambda';\gamma)$ is logarithmically divergent at the critical point $\lambda_c=1$:

$$\frac{\partial\ln d(\lambda,\lambda';\gamma)}{\partial\lambda}=k_1\ln|\lambda-\lambda_c|+\text{constant}, \quad (7)$$

where the prefactor $k_1$ is non-universal in the sense that it depends on $\lambda'$ and $\gamma$. The numerical results are plotted in Fig. 2 for $\lambda'=2$ and $\gamma=1$. The least square method yields $k_1\approx-0.079742$. For systems of finite sizes $L$'s, there are no divergence in the derivatives of $\ln d(\lambda,\lambda';\gamma)$ with respect to $\lambda$, since the second-order QPT only occurs in the thermodynamic limit. Instead, some pronounced peaks occur at the so-called quasi-critical points $\lambda_m$ that approach the critical value as $\lambda_m\sim 1-5.52233L^{-0.99321}$, with the peak values logarith-

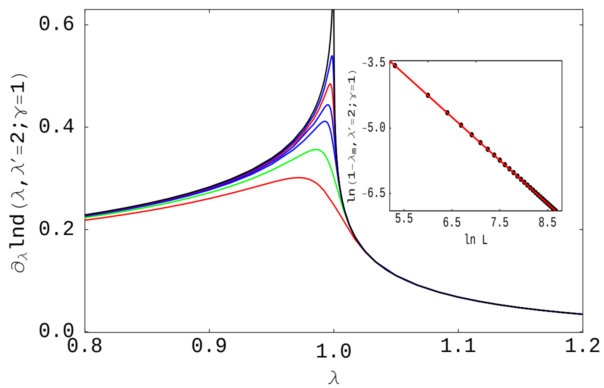


FIG. 2: (color online) Main: the logarithmic divergence near the critical point $\lambda_c = 1$ is analyzed. This is achieved by considering $\partial_\lambda \ln d(\lambda, \lambda' = 2; \gamma = 1)$ as the function of the transverse field strength $\lambda$. The curves shown correspond to different lattice sizes $L = 201, 401, 1201, 2001, 4001, \infty$. The maximum gets more pronounced, with the system size increasing. Inset: the position of maximum approaches the critical point $\lambda_c = 1$ as $\lambda_m \sim 1 - 5.52233L^{-0.99321}$.

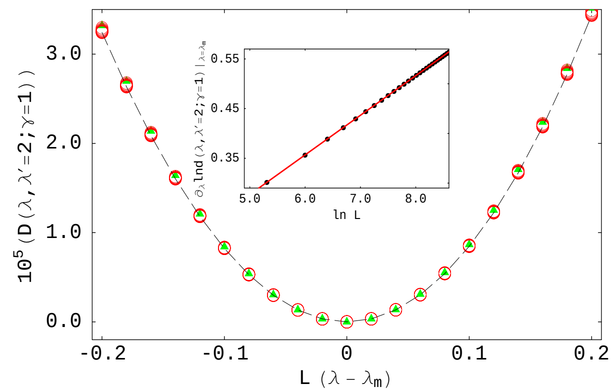


FIG. 3: (color online) Main: a finite size scaling analysis is carried out for a quantity defined as $D(\lambda, \lambda'; \gamma) = 1 - \exp[\partial_\lambda \ln d(\lambda, \lambda'; \gamma) - \partial_\lambda \ln d(\lambda, \lambda'; \gamma)|_{\lambda=\lambda_m}]$. According to the finite size scaling ansatz in the case of logarithmic divergences, one expects that $D(\lambda, \lambda'; \gamma)$ is a function of $L(\lambda - \lambda_m)$. Indeed, all the data from $L = 801$ up to $L = 4001$ collapse on a single curve. This shows that the system at the critical point is scaling invariant (and thus comformally invariant) and that the correlation length critical exponent $\nu$ is 1. Inset: the peak value of $\partial_\lambda \ln d(\lambda, \lambda' = 2; \gamma = 1)$ at $\lambda_m$ diverges as the system size increases, leading to $k_2 \approx 0.0797726$.

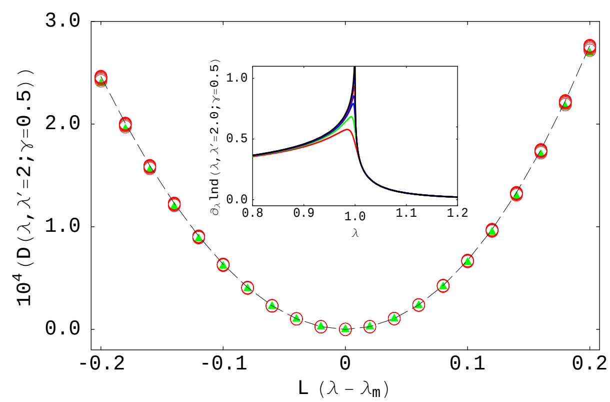


FIG. 4: (color online) The universality hypothesis for the scaling parameter extracted from for the quantum Ising model in a transverse field is checked against different values of $\gamma$ and $\lambda'$. Main: in this case we have chosen $\gamma = 1/2$ and $L$ ranging from 2801 up to 6001. All the data collapse, consistent with the fact that the correlation length critical exponent $\nu$ is 1. The inset shows that the derivative of the logarithmic function of the scaling parameter $d(\lambda, \lambda'; \gamma)$ with respect to $\lambda$ for $\lambda' = 2$ and $\gamma = 1/2$ is logarithmically divergent at $\lambda_c = 1$, with $\lambda_m \sim 1 - 3.23906L^{-1.01135}$.

mically diverging with increasing system size $L$,

$$\frac{\partial \ln d(\lambda, \lambda'; \gamma)}{\partial \lambda}\Big|_{\lambda=\lambda_m} = k_2 \ln L + \text{constant}, \qquad (8)$$

where the non-universal prefactor $k_2$ takes the value $k_2 \approx 0.079773$. The scaling ansatz in the systems exhibiting logarithmic divergences [20] requires that the absolute value of the ratio $k_1/k_2$ is the correlation length critical exponent $\nu$. In this case, $|k_1/k_2| \sim 0.999613$, very close to the exact value 1.

In the case of logarithmic divergences, a proper scaling ansatz has been addressed in Ref. [20]. Taking into account the distance of the maximum of $\partial_\lambda \ln d(\lambda, \lambda'; \gamma)$ from the critical point, we choose to plot $1 - \exp[\partial_\lambda \ln d(\lambda, \lambda'; \gamma) - \partial_\lambda \ln d(\lambda, \lambda'; \gamma)|_{\lambda=\lambda_m}]$ as a function of $L(\lambda - \lambda_m)$ for different system sizes $L$'s. All the data for different $L$'s collapse onto a single curve. The numerical results for the size ranging form $L = 201$ up to $L = 4001$ are plotted in Fig. 3. All these indicates that the system is scaling invariant, i.e., $\xi/L = \xi'/L'$ (and thus conformally invariant), and that the correlation length critical exponent $\nu = 1$.

*Universality.* As is well known, the quantum XY chain belongs to the same quantum Ising universality class for nonzero $\gamma$, with the same critical exponents. To confirm the universality, we need to check the scaling behaviors for different values of $\gamma$. For $\lambda' = 2$ and $\gamma = 1/2$, in the thermodynamic limit, it takes the form (7) with $k_1 \approx -0.157162$, as long as the control parameter is close to the critical point, whereas for a system of finite size, it takes the form (8) with $k_2 \approx 0.157176$. Thus, the absolute value of the ratio $k_1/k_2$ is $|k_1/k_2| = 0.999910$. Fig. 4 shows that all the data for different $L$'s collapse onto a single curve. We also plot the derivative of the logarithmic function of the scaling parameter $d(\lambda, \lambda'; \gamma)$ with respect to $\lambda$ for $\lambda' = 2$ and $\gamma = 1/2$ (see the inset in Fig. 4). All the above results show that the critical exponent $\nu = 1$.

Besides $\gamma$, the scaling parameter $d(\lambda, \lambda'; \gamma)$ also depends on the control parameter $\lambda'$. For $\lambda' = 1/2$ and $\gamma = 1$, in the thermodynamic limit, the derivative of the logarithmic function of the scaling parameter $d(\lambda, \lambda'; \gamma)$ with respect to $\lambda$ still takes the form (7), with $k_1 \approx 0.083005$, as long as the control pa-

rameter is close to the critical point, whereas for a system of finite size, it takes the form (8), with $k_2 \approx -0.083007$. Thus, the absolute value of the ratio $k_2/k_1$ is $|k_2/k_1| = 0.999975$ , again close to the exact value 1. Similarly, all the data for different $L$'s collapse onto a single curve, as shown in Fig. 5. In the inset, we plot the derivative of the logarithmic function of the scaling parameter $d(\lambda, \lambda'; \gamma)$ with respect to $\lambda$ for $\lambda' = 1/2$ and $\gamma = 1$. Therefore, we have demonstrated that the universality hypothesis is valid for the scaling parameter $d(\lambda, \lambda'; \gamma)$.

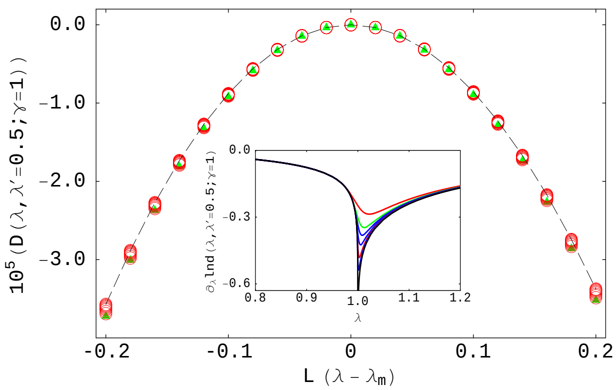


FIG. 5: (color online) The universality for the scaling parameter is checked against different values of $\gamma$ and $\lambda'$. Main: in this case we have chosen $\gamma = 1$ and $L$ ranging from 2801 up to 6001. Consistent with the universality hypothesis for the quantum Ising model in a transverse field, all the data collapse, indicating that the correlation length critical exponent $\nu$ is 1. The inset shows that the derivative of the logarithmic function of the scaling parameter $d(\lambda, \lambda'; \gamma)$ with respect to $\lambda$ for $\lambda' = 1/2$ and $\gamma = 1$ is logarithmically divergent at $\lambda_c = 1$, with $\lambda_m \sim 1 + 3.50186L^{-0.94107}$.

*Discussions and conclusions.* As a basic notion of quantum information science, fidelity may be used to detect QPTs in condensed matter systems. Remarkably, an intimate connection exists between RG flows, QPTs and the scaling parameter which may be extracted from the fidelity [10]. The scaling parameter is well defined in the thermodynamic limit, in sharp contrast to the fidelity itself that always vanishes for continuous QPTs. Different from a bipartite entanglement measure, the fidelity approach does not involve the partition of the whole system into different parts, and the system is treated as a *whole* from the starting point. *In some sense, such a difference may be counted as the contribution from multipartite entanglement*. Therefore one may expect that the fidelity approach possesses significant advantage over the conventional bipartite entanglement approach [21].

Another feature worth to be mentioned is that fidelity is simple to be evaluated in the matrix product state (MPS) representation [10]. On the other hand, many efficient numerical algorithms are now available due to the latest developments in classical simulation of quantum systems [22, 23, 24]. This makes it practical to determine all information including stable and unstable fixed points along RG flows [10], and to extract critical exponents from the scaling parameter, as shown for the quantum Ising model in a transverse field. In this regard, algorithms for periodic boundary conditions [22] and infinite systems [23] are powerful enough to extract meaningful information for critical systems.

In summary, we have performed a finite size scaling analysis for the scaling parameter, whose analytical expression has been extracted from the fidelity for two ground states corresponding to different values of the control parameter for the one-dimensional quantum Ising model in a transverse field near the critical point. In the thermodynamic limit, the logarithmical divergence of the derivative of the scaling parameter with respect to the transverse field strength is demonstrated numerically, consistent with the conformal invariance at the critical point. This makes it possible to extract the correlation length critical exponent. The latter turns out to be universal, in the sense that the correlation length critical exponent thus extracted does not depend on either the anisotropic parameter $\gamma$ or the transverse field strength $\lambda$.

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